SAND2012-7387P

DAKOTA 101

Sensitivity Analysis

http://dakota.sandia.gov/

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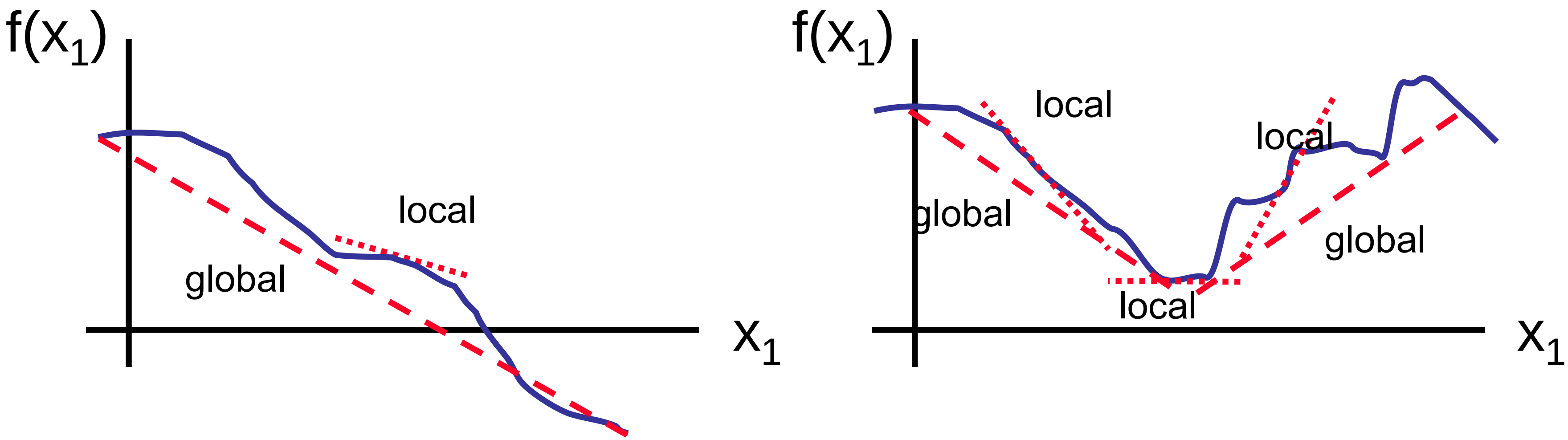
Learning Goals: Sensitivity Analysis

- Define sensitivity analysis, why to apply, potential benefits
- Discuss and share relevant application examples
- Create a DAKOTA study to automate single and joint parameter variations (that you likely already do)
- Perform global sensitivity analysis with DAKOTA's sampling and DACE methods
- Understand DAKOTA outputs, including tabular data file and relevant screen output
- Understand options for SA in DAKOTA and how to choose an approach for your problem

Why Perform Sensitivity Analysis?

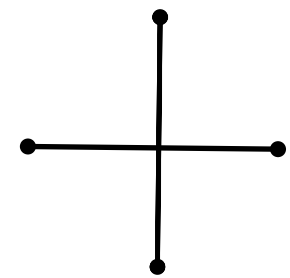
- What? Understand code output variations as input factors vary
- Why? Identify most important variables and their interactions
  - Identify key model characteristics: smoothness, nonlinear trends, robustness
  - Provide a focus for resources
    - Data gathering and model development
    - Code development
    - Uncertainty characterization
  - Screening: Identity the most important variables, down-select for further UQ or optimization analysis
  - Can have the side effect of identifying code and model issues
  - Provide a basis for constructing surrogate models
- DAKOTA SA formalizes and generalizes one-off sensitivity studies you're likely already doing
- Provides richer global sensitivity analysis methods

Sensitivity Analysis:
Influence of Inputs on Outputs



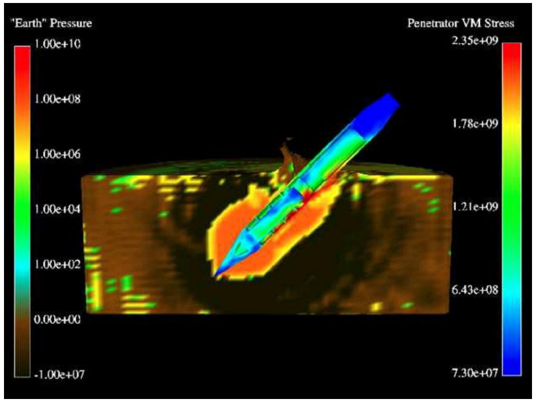
Assess variations in f(x1) due to (small or large) perturbations in x1.

- **Local sensitivities**
  - Partial derivatives at a specific point in input space.
  - Given a specific x1, what is the slope at that point?
  - Can be estimated with finite differences
- **Global sensitivities**
  - Found via sampling and regression.
  - What is the general trend of the function over all values of x1?
  - Typically consider inputs uniformly over their whole range



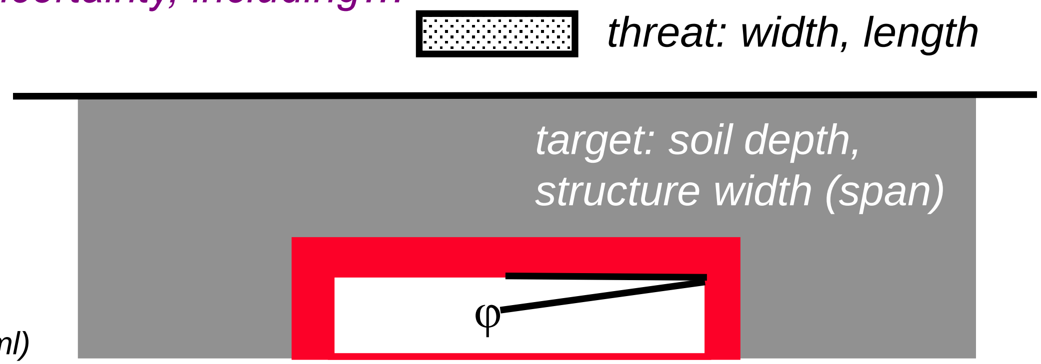
many already do basic SA; perturb from nominal, see effect

Global SA Example: Earth Penetrator

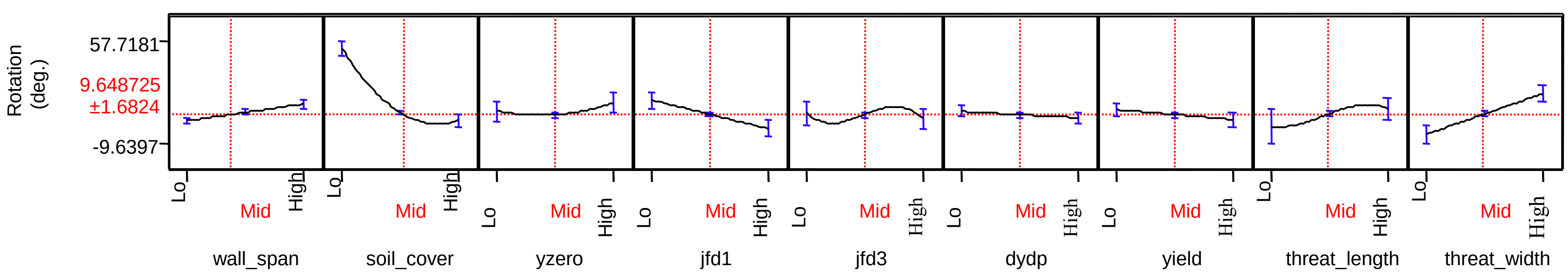


Notional model for illustration purposes only (http://www.sandia.gov/ASC/library/fullsize/penetrator.html)

12 parameters describing target & threat uncertainty, including…

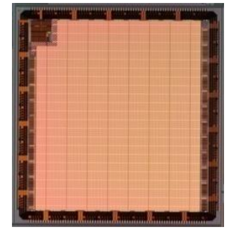


- **Underground target with external threat: assess sensitivity in target response to target construction and threat characteristics**
- **Response: angular rotation (φ) of target roof at mid-span**
- **Analysis: CTH Eulerian shock physics code; JMP stats**
- **Revealed most sensitive input parameters and nonlinear relationships**



Global SA Example: Electrical Circuits

- **CMOS7 ViArray: generic ASIC implementation platform; *applications in NW, satellite, command & control***
- **Modeling and simulation used in design phase to assess predicted performance during photocurrent event, including sensitivity/variability of supply voltage**
- **DAKOTA coupled to Xyce circuit simulator to determine which process layers contributed most to device performance**
- **Analysis outcomes:**
  - **Ranking of component effects on voltages**
  - **Discovery and follow-on discussion of both expected and unexpected sensitive factors**
  - **Automated execution of 1000s of simulation runs, each 2.0h to 4.5h**



	Vdd Metrics	
	node max	node avg
METAL1	0.96	0.82
METAL2	0.11	0.04
METAL3	0.10	0.05
METAL4	0.80	0.81
METAL5	0.86	0.91
VIA1	0.71	0.66
VIA2	0.80	0.76
VIA3	0.57	0.60
VIA4	0.91	0.94
CONTACT	0.21	0.13
polyc	0.04	0.05

correlation coefficients

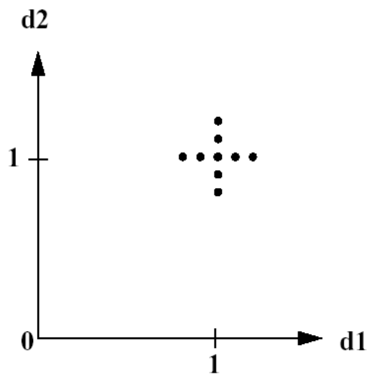
Brief Group Discussion: Current SA Practice

5 min discussion

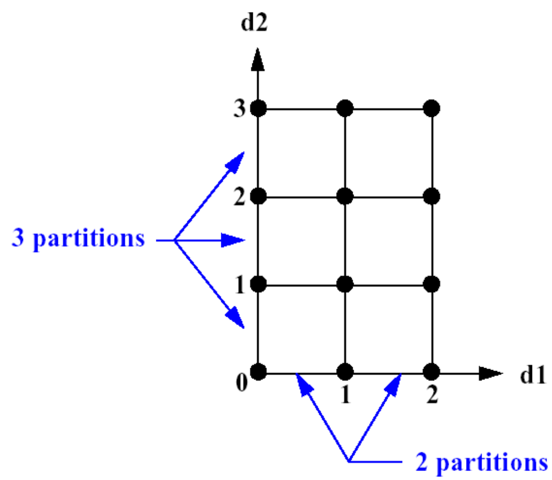
- Do you currently perform sensitivity analysis or parameter perturbations?
- What are example SA questions you ask in your domain?
- How do you answer them currently?
- What measures of sensitivity, ranking, or importance are you most familiar with?
- What are the key challenges you face?

- What are some examples of SA questions you could ask of the cantilever problem?
- What might you expect the results to be?

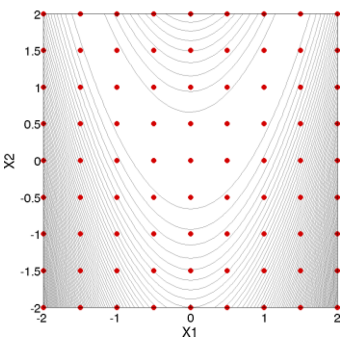
Basic SA in DAKOTA: Parameter Studies



- Start at nominal values, perturb up and down
- Together: perform a DAKOTA centered parameter study on cantilever beam problem
- Convey to DAKOTA the parameter variations and which responses to study
- Example DAKOTA screen output and tabular file



- Group exercise: what would you change in the DAKOTA input to instead perform the grid parameter study at left?
- Use DAKOTA Reference Manual and/or JAGUAR
- What do you see as benefits/drawbacks of these methods?

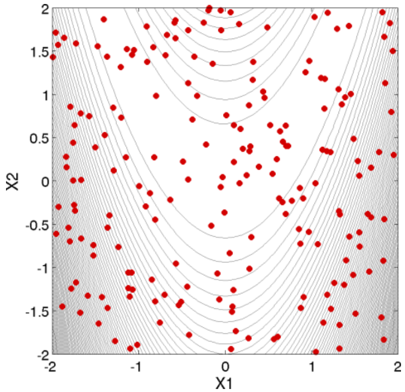


Example: uniform grid over [-2.0, 2.0]

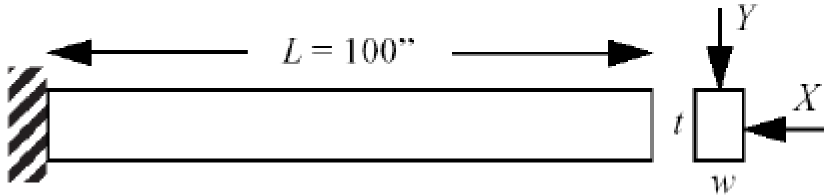
Global SA in DAKOTA

- Global sensitivity analysis aims to assess effect of input variables considered jointly over their whole range. DAKOTA process:
  - Variables: assume inputs fall within lower and upper bounds (uniform assumption for SA)
  - Method: e.g., generate uniform random samples over intervals
  - Responses: compute response value at each sample point
  - Analyze input/output relationships

- Methods: sample designs spanning input space (DACE ~ DOE):
  - Sampling: Monte Carlo, Latin hypercube, Quasi-MC, CVT
  - DOE/DACE: Full-factorial, orthogonal arrays, Box-Behnken, CCD
  - Morris one-at-a-time
- Typical analysis results
  - Simple and partial (including rank) correlation coefficients
  - Regression and resulting coefficients
  - Variance-based decomposition
  - Importance factors



Cantilever Beam Analysis Problem



- **What are some global sensitivity analysis questions you could ask for the cantilever beam?**
- **What kinds of bounds or variable characterizations would you use?**
- **Beam computational model:**

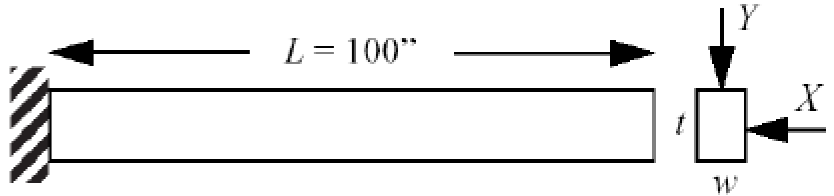
weight (*area* = *w*t*)**

$$stress = \frac{600}{wt^2}Y + \frac{600}{w^2t}X \le R$$

$$displacement = \frac{4L^3}{Ewt}\sqrt{\left(\frac{Y}{t^2}\right)^2 + \left(\frac{X}{w^2}\right)^2} \le D_0$$

Given values of *w, t, R, E, X, Y,* DAKOTA's `mod_cantilever` driver computes *area, stress-R, displacement-D_0*

Cantilever Beam Analysis Problem



- **Example sensitivity analysis goals:**
  - **Determine influence of beam_width, beam_thickness, R (yield stress), E (Young’s modulus), X (horizontal load), Y (vertical load) on each of area (weight), stress, and displacement**
  - **Determine whether these have only a main effect or if parameter interactions and higher order effects figure in**

weight (*area = w*t*)

$$stress = \frac{600}{wt^2} Y + \frac{600}{w^2 t} X \leq R$$

$$displacement = \frac{4L^3}{Ewt} \sqrt{\left(\frac{Y}{t^2}\right)^2 + \left(\frac{X}{w^2}\right)^2} \leq D_0$$

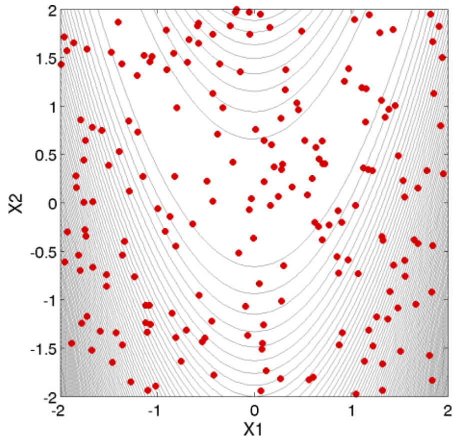
Given values of *w, t, R, E, X, Y,* DAKOTA’s `mod_cantilever` driver computes *area, stress-R, displacement-D_0*

Exercise: Determine trends relative to parameters for cantilever problem

- Use JAGUAR to construct and run a sampling method to determine most influential parameters for cantilever (as evaluated by `mod_cantilever` analysis driver)
- 6 uniform variables with descriptors:

Variable	R	E	X	Y	beam_width	beam_thickness
Upper bound	48000	4.50E+07	700	1200	2.2	2.2
Lower Bound	32000	1.50E+07	300	800	2	2

- Cantilever has 3 response functions, instead of 1; specify descriptors `‘area’ ‘stress’ ‘displacement’`
- 100 samples
- Could start with `dakota_rosenbrock_nond.in` (SA UQ Sampling in JAGUAR)
- See DAKOTA reference manual: method, variables, responses commands (http://dakota.sandia.gov/documentation.html)
- Review DAKOTA output to examine correlations (simple, partial, rank)



Potential Solution:
Sensitivity Analysis for Cantilever

```
# DAKOTA INPUT FILE - extraexamples/dakota_sa_cantilever.in
strategy,
    single_method
    tabular_graphics_data
method,
    sampling
    sample_type lhs
    seed =52983
    samples = 100
variables,
    uniform_uncertain = 6
      upper_bounds   48000   45.E+6  700.   1200.  2.2    2.2
      lower_bounds    32000.   15.E+6  300.    800.   2.0     2.0
      descriptors  'R' 'E' 'X' 'Y' 'beam_width' 'beam_thickness'
interface,
    direct
    analysis_driver = 'mod_cantilever'
responses,
    num_response_functions = 3
    response_descriptors = 'weight' 'stress' 'displ'
    no_gradients
    no_hessians
```

Exercise: Determine trends relative to parameters for cantilever problem

- **Review correlations in DAKOTA output**
  - **Simple correlation:** measures the strength and direction of a linear relationship between variables
  - **Partial correlation:** like simple correlation but adjusts for the effects of the other variables
  - **Rank correlations:** simple and partial correlations performed on "rank" of data

```
Partial Correlation Matrix between input and output:
                       weight        stress         displ
            R  1.36556e-01 -9.89955e-01 -5.82547e-02
            E -2.59807e-02  1.51530e-02 -9.53598e-01
            X -8.58158e-03  9.96167e-01  3.12725e-01
            Y  5.15226e-02  9.96214e-01  7.35493e-01
            w  9.99659e-01 -9.84197e-01 -4.20681e-01
            t  9.99659e-01 -9.89246e-01 -5.24940e-01
```

Correlation near:

0, no relationship

1, strong positive relationship (as x increases, y increases)

-1, strong negative relationship (as x increases, y decreases)

Summary Results: Correlations for Cantilever

Simple Correlation Matrix

	R	*E*	*X*	*Y*	beam width	beam thickness	*weight*	*stress*	*displ*
R	1.000								
E	-0.022	1.000							
X	0.012	-0.007	1.000						
Y	0.020	0.017	-0.027	1.000					
beam width	0.009	-0.009	-0.017	-0.014	1.000				
beam thickness	0.003	-0.013	0.038	-0.025	-0.012	1.000			
weight	0.011	-0.016	0.014	-0.027	0.703	0.703	1.000		
stress	-0.345	0.022	0.557	0.579	-0.303	-0.339	-0.457	1.000	
displ	0.009	-0.879	0.085	0.293	-0.125	-0.164	-0.207	0.313	1.000

Partial Correlation Matrix between Input and Output:

	weight	**stress**	**displ**
R	0.137	-0.990	-0.058
E	-0.026	0.015	-0.954
X	-0.009	0.996	0.313
Y	0.052	0.996	0.735
beam_width	1.000	-0.984	-0.421
beam_thickness	1.000	-0.989	-0.525

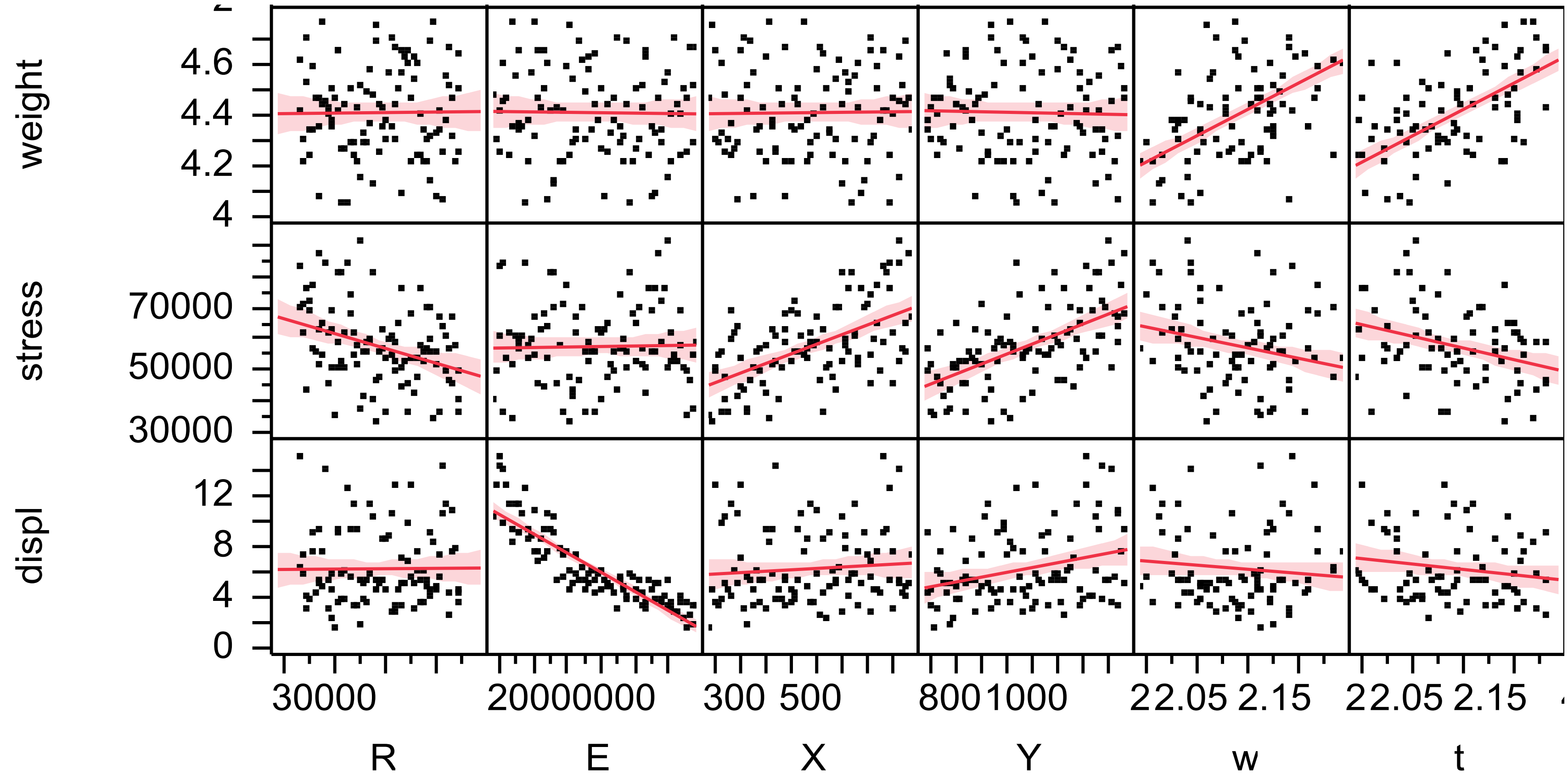
Partial Rank Correlation Matrix between Input and Output:

	weight	**stress**	**displ**
R	-0.071	-0.837	-0.056
E	0.082	-0.085	-0.981
X	0.179	0.924	0.531
Y	-0.055	0.934	0.824
beam_width	0.981	-0.800	-0.559
beam_thickness	0.980	-0.838	-0.753

Beam width and thickness are important contributors to all outputs, several other variables also rate highly on partial correlations.

Results: Input/Output Scatter Plots for Cantilever

The `dakota_tabular.dat` file can be used in Mintab, JMP, Excel, etc., to generate scatter plots



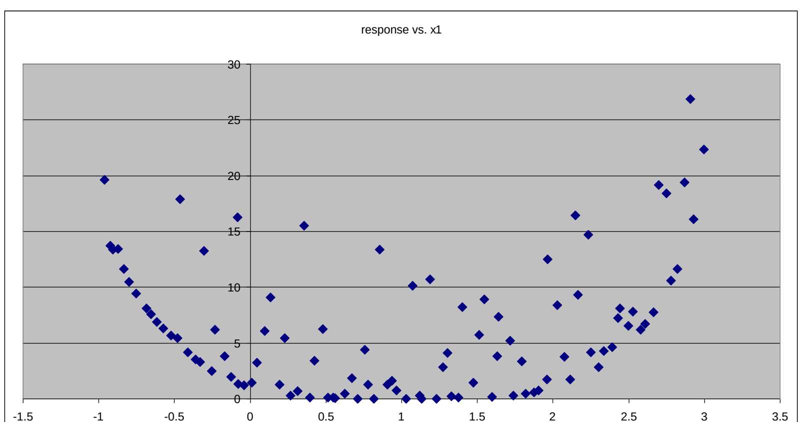
Group discussion

- What is expected, limited about this approach?
- What approaches would you take?
- What assumptions are we making? How would changing them affect results?
- Investigate another DAKOTA method in the reference manual. Understand how to specify…

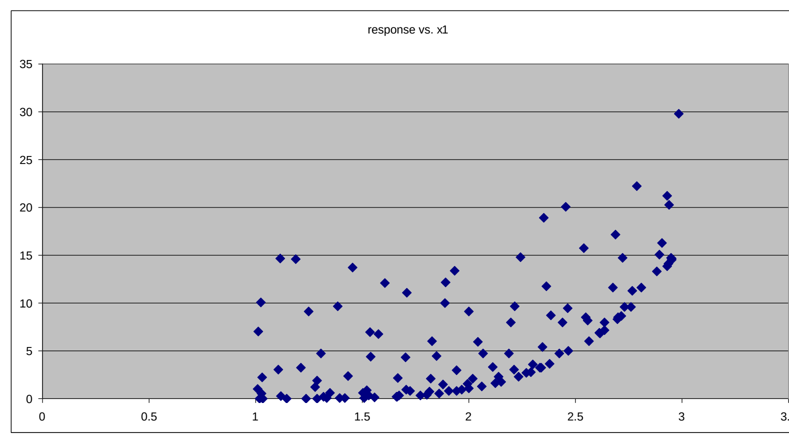
SA Assumptions and Pitfalls

- Global sensitivity analysis sensitive to range, distribution choices
- Some methods generate orthogonal designs, some do not; affects ability to separate effects of different variables
- Question the results: correlation coefficients or low-order models can mislead
- Example: scatterplots for “textbook” problem, different bounds:

Bounds = [-1, 3]



Bounds = [1, 3]



Optional: Additional Sensitivity Analysis Capabilities

- **Variance-based decomposition (via sampling or PCE)**
  - **Goal: Apportion uncertainty in responses to uncertainty in inputs**
  - **Expensive: K*(N+2) simulations required, K = # samples, N = # variables, recommended K ≥ 100**
  - **Exercise: Modify the sensitivity analysis method to perform variance-based decomposition on the cantilever problem**

- **Main Effects/Analysis of Variance (ANOVA)**
  - **Goal: Determine effect of a variable on mean behavior**
  - **Uses design of experiments: Coverage of space (e.g., space filling, interior, boundaries/extremes, etc.) varies by design**
  - **Exercise: Modify the sensitivity analysis method to perform a main effects analysis using an orthogonal array on the cantilever problem**

Exercise: Explore Other SA Methods for Cantilever

```
method,
sampling
   sample_type lhs
   seed =52983
   samples = 100
```

LHS Sampling

```
method,
   dace oas
   main_effects
   seed =52983
   samples = 500
```

Main Effects Analysis using Orthogonal Arrays

```
method,
sampling
   sample_type lhs
   seed =52983
   samples = 500
   variance_based_decomp
```

Variance-based Decomposition using LHS Sampling

```
method,
   psuade_moat
   partitions = 3
   seed =52983
   samples = 100
```

Morris One-At-a-Time

Same input file, just change method.

Results for VBD and Main Effects

Global sensitivity indices for each response function:			
weight	Sobol	indices:	
	Main	Total	
	0.00	0.00	**R**
	0.00	0.00	**E**
	0.00	0.00	**X**
	0.00	0.00	**Y**
	0.49	0.51	**beam_width**
	0.51	0.52	**beam_thickness**
stress	**Sobol**	**indices:**	
	Main	**Total**	
	0.16	0.13	**R**
	0.00	0.00	**E**
	0.37	0.36	**X**
	0.39	0.36	**Y**
	0.08	0.08	**beam_width**
	0.11	0.12	**beam_thickness**
displ	**Sobol**	**indices:**	
	Main	**Total**	
	0.00	0.00	**R**
	0.90	0.92	**E**
	0.02	0.02	**X**
	0.07	0.08	**Y**
	0.02	0.01	**beam_width**
	0.04	0.05	**beam_thickness**

Variance-based decomposition

Response Function 1

ANOVA	Table	for	Factor	(Variable)	4	
Source	of	Sum	of	Mean	Sum	
Variation	DoF	Squares	of	Squares	Fdata	
Between	Groups	22	2.18E-03	9.89E-05	**3.22E-03**	**Y**
Within	Groups	506	1.55E+01	3.07E-02		
Total	528	1.55E+01				
ANOVA	Table	for	Factor	(Variable)	5	
Source	of	Sum	of	Mean	Sum	
Variation	DoF	Squares	of	Squares	Fdata	
Between	Groups	22	7.80E+00	3.55E-01	**2.32E+01**	**Beam Width**
Within	Groups	506	7.73E+00	1.53E-02		
Total	528	1.55E+01				
ANOVA	Table	for	Factor	(Variable)	6	
Source	of	Sum	of	Mean	Sum	
Variation	DoF	Squares	of	Squares	Fdata	
Between	Groups	22	7.70E+00	3.50E-01	**2.26E+01**	**Beam Thickness**
Within	Groups	506	7.84E+00	1.55E-02		
Total	528	1.55E+01				

Main Effects Analysis

Same relative ranking across methods.

DAKOTA Sensitivity Analysis Summary

- **What? Understand code output variations as input factors vary; main effects and key parameter interactions.**
- **Why? Identify most important variables and their interactions**
- **How? What DAKOTA methods are relevant? What results?**

Category	DAKOTA method names	univariate trends	correlations	modified mean, s.d.	main effects Sobol inds.	importance factors / local sensis
Parameter studies	`centered, vector, list`	P				
	`grid`		D		P	
Sampling	**`sampling`**`, dace lhs, dace random, fsu_quasi_mc, fsu_cvt`	P	D			
	`with variance_based_decomp...`				D	
DACE (DOE-like)	`dace {oas, oa_lhs, box_behnken, central_composite}`		D		D	
MOAT	`psuade_moat`			D		
PCE, SC	`polynomial_chaos, stoch_collocation`				D	D
Mean value	`local_reliability`					D

multi-purpose!

D: DAKOTA
P: Post-processing (3rd party tools)

- **Also see DAKOTA Usage Guidelines in User's Manual**

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SA References

- Saltelli A., Ratto M., Andres T., Campolongo, F., et al., Global Sensitivity Analysis: The Primer, Wiley, 2008.
- J. C. Helton and F. J. Davis. Sampling-based methods for uncertainty and sensitivity analysis. Technical Report SAND99-2240, Sandia National Laboratories, Albuquerque, NM, 2000.
- Sacks, J., Welch, W.J., Mitchell, T.J., and Wynn, H.P. Design and analysis of computer experiments. Statistical Science 1989; 4:409–435.
- Oakley, J. and O'Hagan, A. Probabilistic sensitivity analysis of complex models: a Bayesian approach. J Royal Stat Soc B 2004; 66:751–769.

- **DAKOTA User's Manual**
  - Parameter Study Capabilities
  - Design of Experiments Capabilities/Sensitivity Analysis
  - Uncertainty Quantification Capabilities (for MC/LHS sampling)
- Corresponding Reference Manual sections

Learning Goals Revisited: Sensitivity Analysis

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